

Relativistic Hartree-Bogoliubov theory in coordinate space: finite element solution for a nuclear system with spherical symmetry

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Abstract

A C++ code for the solution of the relativistic Hartree-Bogoliubov theory in coordinate space is presented. The theory describes a nucleus as a relativistic system of baryons and mesons. The RHB model is applied in the self-consistent mean-field approximation to the description of ground state properties of spherical nuclei. Finite range interactions are included to describe pairing correlations and the coupling to particle continuum states. Finite element methods are used in the coordinate space discretization of the coupled system of Dirac-Hartree-Bogoliubov integro-differential eigenvalue equations, and Klein-Gordon equations for the meson fields. The bisection method is used in the solution of the resulting generalized algebraic eigenvalue problem, and the biconjugate gradient method for the systems of linear and nonlinear algebraic equations, respectively.

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PROGRAM SUMMARY

Title of program: spnRHBfem.cc

Catalogue number:

Program obtainable from:

Computer for which the program is designed and others on which it has been tested: any Unix work-station.

Operating system: Unix

Programming language used: C++

No. of lines in combined program and test deck:

Keywords: relativistic Hartree-Bogoliubov theory, mean-field approximation, spherical nuclei, pairing, Dirac-Hartree-Bogoliubov equations, Klein-Gordon equation, Finite Element Method, bisection method, classes

Nature of physical problem

The ground-state of a spherical nucleus is described in the framework of relativistic Hartree-Bogoliubov theory in coordinate space. The model describes a nucleus as a relativistic system of baryons and mesons. Nucleons interact in a relativistic covariant manner through the exchange of virtual mesons: the isoscalar scalar σ -meson, the isoscalar vector ω -meson and the isovector vector ρ -meson. The model is based on the one boson exchange description of the nucleon-nucleon interaction. Pairing correlations are described by finite range Gogny forces.

Method of solution

An atomic nucleus is described by a coupled system of partial integro-differential equations for the nucleons (Dirac-Hartree-Bogoliubov equations), and differential equations for the meson and photon fields (Klein-Gordon equations). A method is presented which allows a simple, self-consistent solution based on finite element analysis. Using a formulation based on weighted residuals, the coupled system of Dirac-Hartree-Bogoliubov and Klein-Gordon equations is transformed into a generalized algebraic eigenvalue problem, and systems of linear and nonlinear algebraic equations, respectively. Finite elements of arbitrary order are used on adaptive non-uniform radial mesh. The generalized eigenvalue problem is solved in narrow windows of the eigenparameter using a highly efficient bisection method for band matrices. A biconjugate gradient method is used for the solution of systems of linear and nonlinear algebraic equations.

Restrictions on the complexity of the problem

In the present version of the code we only consider nuclear systems with spherical symmetry.

LONG WRITE-UP

1 Introduction

Relativistic mean-field theory has been extensively applied in calculations of nuclear matter and properties of finite nuclei throughout the periodic table. The theory provides a framework for describing the nuclear many-body problem as a relativistic system of baryons and mesons [1, 2, 3]. In the self-consistent mean-field approximation, detailed calculations have been performed for a variety of nuclear structure phenomena (for a recent review see [4]). More recently, the relativistic mean-field model has been also applied in the description of the structure of exotic nuclei with extreme isospin values. This new field includes many interesting phenomena: extremely weak binding of the outermost nucleons, coupling between bound states and the particle continuum, regions of neutron halos with very diffuse neutron densities, large spatial dimensions and the existence of the neutron skin. Major modifications of shell structures in drip-line nuclei have been predicted, as well as modifications in the onset and evolution of collectivity. For most phenomena along the line of stability, non-relativistic models and the relativistic framework predict very similar results, although relativistic mean-field models provide a more economical description. For drip-line nuclei, on the other hand, one also expects differences in the predictions of non-relativistic and relativistic models, especially in the treatment of the spin-orbit interaction [4].

In drip-line nuclei the Fermi level is found close to the particle continuum. The lowest particle-hole or particle-particle modes are often embedded in the continuum, and the coupling between bound and continuum states has to be taken into account explicitly. In the mean-field approximation the most important residual interaction is the pairing force. Therefore, in the description of ground-state properties, it is essential to include mean-field and pairing correlations simultaneously. The Relativistic Hartree-Bogoliubov (RHB) theory in coordinate space, which is an extension of non-relativistic HFB-theory [5], provides such a unified description. In particular, it includes the scattering of nucleonic pairs from bound states to the positive energy continuum. The RHB theory has recently been applied in the description of ground-state properties of Sn and Pb isotopes [6], using an expansion in a large oscillator basis for the solution of the Dirac-Hartree-Bogoliubov equations. In many applications an expansion of the wave functions in an appropriate oscillator basis of spherical or axial symmetry provides a satisfactory level of accuracy. However, in the case of drip-line nuclei, the expansion in the localized oscillator basis presents only a poor approximation to the continuum states, and the convergence of such expansions is too slow and is not uniform. Examples are exotic phenomena such as neutron halos and neutron skins. In order to correctly describe the coupling between bound and continuum states, the Dirac-Hartree-Bogoliubov equations have to be solved in coordinate space. Discretization in coordinate space provides also the advantage that exotic shapes and/or large deformations can be described, without preparing a basis specific to each deformation. Recently, a fully self-consistent RHB model in coordinate space has been used to describe the two-neutron halo in ^{11}Li [7]. However, only a density dependent force

of zero range has been used in the pairing channel. In general, it is assumed that a finite range interaction would provide a more realistic description of pairing correlations. In the present article we describe a C++ code which can be used to calculate ground state properties of spherical nuclei, within the framework of RHB theory in coordinate space, with finite range forces in the pairing channel.

A convenient procedure for the coordinate space discretization of the Dirac-Hartree-Bogoliubov equations is provided by Finite Element Methods (FEM) [8, 9, 10, 11]. In Refs. [12, 13] we have applied FEM to the solution of the coupled system of relativistic mean-field equations in the description of a one-dimensional slab of nuclear matter and of spherical doubly closed-shell nuclei. We have investigated the applicability of FEM in the calculation of bound and continuum eigenstates of the Dirac equation. Since the spectrum of the hamiltonian of the hyperbolic Dirac equation is not bounded from below, finite element methods cannot be applied in the variational formulation. The method of weighted residuals produces element matrix integral definitions that would be identical to those obtained from a variational form, if one existed. Our analysis has shown that FEM provide very accurate solutions for the relativistic eigenvalue problem in the self-consistent mean-field approximation. In the present work we extend the model to include pairing correlations in the framework of RHB theory.

The article is organized as follows. In Sec. 2 the Relativistic Hartree-Bogoliubov theory is described. Dirac-Hartree-Bogoliubov equations for a system with spherical symmetry are derived. The finite element analysis is described in Sec. 3. In Sec. 4 we present some illustrative calculations and discuss the quality of our approximations and numerical results. The structure of the C++ code is described in Sec. 5.

2 The relativistic Hartree-Bogoliubov equations

The Hartree-Fock-Bogoliubov (HFB) theory provides a unified description of mean-field and pairing correlations in nuclei [14]. Independent quasiparticles are introduced and the ground state of a nucleus $|\Phi\rangle$ is represented as the vacuum with respect to these quasiparticles. The quasi-particle operators are defined by a unitary Bogoliubov transformation of the single-nucleon creation and annihilation operators. The generalized single-particle hamiltonian of HFB theory contains two average potentials: the self-consistent field $\hat{\Gamma}$ which encloses all the long range ph correlations, and a pairing field $\hat{\Delta}$ which sums up the pp -correlations. The expectation value of the nuclear hamiltonian $\langle\Phi|\hat{H}|\Phi\rangle$ can be expressed as a function of the hermitian density matrix ρ , and the antisymmetric pairing tensor κ . The variation of the energy functional with respect to ρ and κ produces the single quasi-particle Hartree-Fock-Bogoliubov equations (for details of the derivation we refer to [14]).

$$\begin{pmatrix} \hat{h} - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h} + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}. \quad (1)$$

HFB-theory, being a variational approximation, results in a violation of basic symmetries of the nuclear system, among which the most important is the nonconservation of the number of particles. In order that the expectation value of the particle number operator in the ground state equals the number of nucleons, equations (1) contain a chemical potential λ which has to be determined by the particle number subsidiary condition. The column vectors denote the quasi-particle wave functions, and E_k are the quasi-particle energies.

The relativistic extension of the HFB theory is described in Ref. [15]. In the Hartree approximation for the self-consistent mean field, the Relativistic Hartree-Bogoliubov (RHB) equations read

$$\begin{pmatrix} \hat{h}_D - m - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D + m + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}. \quad (2)$$

where \hat{h}_D is the single-nucleon Dirac hamiltonian [13], and m is the nucleon mass. The RHB equations are non-linear integro-differential equations. They have to be solved self-consistently, with potentials determined in the mean-field approximation from solutions of Klein-Gordon equations for mesons [13]

$$[-\Delta + m_\sigma^2] \sigma(\mathbf{r}) = -g_\sigma \rho_s(\mathbf{r}) - g_2 \sigma^2(\mathbf{r}) - g_3 \sigma^3(\mathbf{r}) \quad (3)$$

$$[-\Delta + m_\omega^2] \omega^0(\mathbf{r}) = -g_\omega \rho_v(\mathbf{r}) \quad (4)$$

$$[-\Delta + m_\rho^2] \rho^0(\mathbf{r}) = -g_\rho \rho_3(\mathbf{r}) \quad (5)$$

$$-\Delta A^0(\mathbf{r}) = e \rho_p(\mathbf{r}). \quad (6)$$

for the sigma meson, omega meson, rho meson and photon field, respectively. The spatial componenets ω , ρ , and \mathbf{A} vanish due to time reversal symmetry. Because of charge conservation, only the 3-component of the isovector rho meson contributes. The source terms in equations (3) to (6) are sums of bilinear products of baryon amplitudes

$$\rho_s = \sum_{E_k > 0} V_k^\dagger \gamma^0 V_k, \quad (7)$$

$$\rho_v = \sum_{E_k > 0} V_k^\dagger V_k, \quad (8)$$

$$\rho_3 = \sum_{E_k > 0} V_k^\dagger \tau_3 V_k, \quad (9)$$

$$\rho_{\text{em}} = \sum_{E_k > 0} V_k^\dagger \frac{1 - \tau_3}{2} V_k. \quad (10)$$

where the sums run over all positive energy states. For M degrees of freedom, for example number of nodes on a radial mesh, the HB equations are $2M$ -dimensional and have $2M$ eigenvalues and eigenvectors. To each eigenvector (U_k, V_k) with eigenvalue E_k , there corresponds an eigenvector (V_k^*, U_k^*) with eigenvalue $-E_k$. Since baryon quasi-particle operators satisfy fermion commutation relations, it is forbidden to occupy the levels E_k and $-E_k$ simultaneously. Usually one chooses the M positive eigenvalues E_k for the solution that corresponds to a ground state of a nucleus with even particle number.

The system of equations (2), and (3) to (6), is solved self-consistently in coordinate space by discretization on the finite element mesh. In the coordinate space representation of the pairing field $\hat{\Delta}$ in (2), the kernel of the integral operator is

$$\Delta_{ab}(\mathbf{r}, \mathbf{r}') = \frac{1}{2} \sum_{c,d} V_{abcd}(\mathbf{r}, \mathbf{r}') \kappa_{cd}(\mathbf{r}, \mathbf{r}'). \quad (11)$$

where a, b, c, d denote all quantum numbers, apart from the coordinate \mathbf{r} , that specify the single-nucleon states. $V_{abcd}(\mathbf{r}, \mathbf{r}')$ are matrix elements of a general two-body pairing interaction, and the pairing tensor is defined as

$$\kappa_{cd}(\mathbf{r}, \mathbf{r}') := \sum_{E_k > 0} U_{ck}^*(\mathbf{r}) V_{dk}(\mathbf{r}'). \quad (12)$$

The integral operator $\hat{\Delta}$ acts on the wave function $V_k(\mathbf{r})$:

$$(\hat{\Delta}V_k)(\mathbf{r}) = \sum_b \int d^3r' \Delta_{ab}(\mathbf{r}, \mathbf{r}') V_{bk}(\mathbf{r}'). \quad (13)$$

The eigensolutions of Eq. (2) form a set of orthogonal (normalized) single quasi-particle states. The corresponding eigenvalues are the single quasi-particle energies. The Bogoliubov transformation from the single-particle coordinate basis of δ -functions to the basis of quasi-particle states is given by the matrix $W_{k\mathbf{r}} := (U_k^T(\mathbf{r}), V_k^T(\mathbf{r}))^T$. \mathbf{r} and k are column and row indices, respectively. In the self-consistent iteration procedure we work in the basis of quasi-particle states. The self-consistent quasi-particle eigenspectrum is then transformed into the canonical basis of single-particle states. The canonical basis is defined to be the one in which the matrix $R_{kk'} = \langle V_k(\mathbf{r}) | V_{k'}(\mathbf{r}) \rangle$ is diagonal. The transformation to the canonical basis determines the energies and occupation probabilities of single-particle states, that correspond to the self-consistent solution for the ground state of a nucleus. In order to determine the canonical basis, we have two possibilities: either diagonalize the density matrix, or diagonalize the matrix

$$R_{kk'} := \langle V_k(\mathbf{r}) | V_{k'}(\mathbf{r}) \rangle \quad (14)$$

Although both methods are in principle equivalent, for numerical reasons we chose the second method, i.e. we diagonalize the matrix $R_{kk'}$. Because of the truncation in quasi-particle space, the dimension of the matrix $R_{kk'}$, which is a matrix in quasiparticle space, is considerably smaller than the dimension of the density matrix in coordinate space.

The transformations from the general single-particle basis to the basis of quasi-particle states, and the canonical basis are illustrated in Fig. 1. The quasi-particle operators and basis states are defined

$$\begin{pmatrix} \hat{a}_k \\ \hat{a}_k^\dagger \end{pmatrix} = \int d^3r \begin{pmatrix} U_{k,\mathbf{r}}^* & V_{k,\mathbf{r}}^* \\ V_{k,\mathbf{r}} & U_{k,\mathbf{r}} \end{pmatrix} \begin{pmatrix} \hat{\Psi}(\mathbf{r}) \\ \hat{\Psi}^\dagger(\mathbf{r}) \end{pmatrix}, \quad \begin{pmatrix} \Phi_U(\mathbf{r}) \\ \Phi_V(\mathbf{r}) \end{pmatrix} = \int_{\mathbf{R}^3} d^3r' \begin{pmatrix} U_{k,\mathbf{r}'} \\ V_{k,\mathbf{r}'} \end{pmatrix} \delta(\mathbf{r} - \mathbf{r}'). \quad (15)$$

The operators in the canonical basis are

$$\begin{pmatrix} \hat{c}_k \\ \hat{c}_k^\dagger \end{pmatrix} = \int d^3r \begin{pmatrix} \psi_k(\mathbf{r}) & 0 \\ 0 & \psi_k^*(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \hat{\Psi}(\mathbf{r}) \\ \hat{\Psi}^\dagger(\mathbf{r}) \end{pmatrix}, \quad \psi_k(\mathbf{r}) = \int_{\mathbf{R}^3} d^3r' \Psi_{k,\mathbf{r}'} \delta(\mathbf{r} - \mathbf{r}'), \quad (16)$$

and the transformation from the quasi-particle to the canonical basis reads

$$\begin{pmatrix} \hat{c}_k \\ \hat{c}_k^\dagger \end{pmatrix} = \sum_{k'} \begin{pmatrix} u_{kk'} & v_{kk'} \\ -v_{kk'} & u_{kk'} \end{pmatrix} \begin{pmatrix} \hat{a}_{k'} \\ \hat{a}_{k'}^\dagger \end{pmatrix}, \quad \psi_k(\mathbf{r}) = \sum_{k'} C_{k'k} \Phi_{V,k'}(\mathbf{r}) \quad (17)$$

The matrix representation of the unitary Bogoliubov transformation \mathbf{W} can be decomposed into a product of three matrices [14]

$$\mathbf{W} = \begin{pmatrix} \mathbf{D} & 0 \\ 0 & \mathbf{D}^* \end{pmatrix} \begin{pmatrix} \bar{\mathbf{U}} & \bar{\mathbf{V}} \\ -\bar{\mathbf{V}} & \bar{\mathbf{U}} \end{pmatrix} \begin{pmatrix} \mathbf{C} & 0 \\ 0 & \mathbf{C}^* \end{pmatrix}. \quad (18)$$

The diagonalization of the matrix $R_{kk'} := \langle V_k(\mathbf{r}) | V_{k'}(\mathbf{r}) \rangle$ produces the unitary matrix \mathbf{C} . Columns of \mathbf{C} are eigenvectors of $R_{kk'}$. The matrices $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}}$ are constructed from the

eigenvalues v_k^2 of $R_{kk'}$

$$\bar{\mathbf{U}} = \begin{pmatrix} u_1 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & & & & \\ \cdot & & \cdot & & & \cdot \\ \cdot & & & u_k & & \cdot \\ \cdot & & & & \cdot & \cdot \\ 0 & & & & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot & 0 & u_N \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{V}} = \begin{pmatrix} v_1 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & & & & \\ \cdot & & \cdot & & & \cdot \\ \cdot & & & v_k & & \cdot \\ \cdot & & & & \cdot & \cdot \\ 0 & & & & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot & 0 & v_N \end{pmatrix} \quad (19)$$

where $u_k = \sqrt{1 - v_k^2}$, and N is the number of solutions. The matrix \mathbf{C} transforms the basis of quasi-particle states into the canonical basis

$$\psi_k(\mathbf{r}) = \sum_{k'} C_{k'k} V_{k'}(\mathbf{r}). \quad (20)$$

The matrix $\mathbf{D} := [\psi_k(\mathbf{r})]$ represents a transformation between two single-particle bases. $\mathbf{E} := \text{diag}(E_k)$ defines the diagonal matrix of quasi-particle energies. In the basis of quasi-particle states the hamiltonian matrix has the diagonal form $\text{diag}(\mathbf{E}, -\mathbf{E})$. The hamiltonian matrix in the single-particle canonical basis is defined by the transformation

$$\mathbf{H} := \begin{pmatrix} \bar{\mathbf{U}} & \bar{\mathbf{V}} \\ -\bar{\mathbf{V}} & \bar{\mathbf{U}} \end{pmatrix} \begin{pmatrix} \mathbf{C} & 0 \\ 0 & \mathbf{C}^* \end{pmatrix} \begin{pmatrix} \mathbf{E} & 0 \\ 0 & -\mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{C}^\dagger & 0 \\ 0 & \mathbf{C}^T \end{pmatrix} \begin{pmatrix} \bar{\mathbf{U}} & -\bar{\mathbf{V}} \\ \bar{\mathbf{V}}^\dagger & \bar{\mathbf{U}}^\dagger \end{pmatrix}. \quad (21)$$

The single-particle energies correspond to the diagonal matrix elements $\varepsilon_n = H_{nn} + \lambda$, where λ denotes the chemical potential. In Fig. 2 we display a schematic single-nucleon spectrum in the relativistic mean-field potential of a finite nucleus. On the left hand side the eigenspectrum of a Dirac hamiltonian is shown. The single-particle hamiltonian corresponds to the average mean-field potential, and the Dirac equation is solved in the Hartree mean-field, and *no-sea* approximations. A Dirac gap is observed between states of negative and positive energy. In vacuum, this gap equals two times the nucleon mass. In a nucleus the Dirac gap extends between the sum and the difference of the scalar sigma-meson potential and vector omega-meson potential. The sum and the difference are given relative to $+m$ and $-m$, respectively. In the center of Fig. 2 the eigenspectrum of the Dirac hamiltonian is shifted by the nucleon mass m . As a result, bound single-nucleon levels have negative energies, while the positive energy domain contains only single-nucleon continuum states. The single quasi-particle spectrum which results as a solution of the relativistic Hartree-Bogoliubov equations is shown on the right hand side of Fig. 2. The number of solutions is two times the number of physical states. As already described, for each eigenvector (U_k, V_k) with energy E_k , the corresponding state (V_k^*, U_k^*) is found at $-E_k$.

In practical calculations the Dirac-Hartree-Bogoliubov and Klein-Gordon equations are discretized on a finite domain \mathcal{D} in coordinate space (indicated by r_{max} in Fig. 2), and the generalized eigenvalue problem is solved in the window $\mathcal{E} := [0, E_{max}]$ of the eigenparameter E . The domain $\mathcal{D} \otimes \mathcal{E}$ is indicated by the shaded area in the right hand side spectrum. By increasing the coordinate space domain the HB spectrum becomes denser, and thus provides a better approximation for the continuum. Larger values of E_{max} take into account couplings to highly excited quasi-particle states. \mathcal{D} and \mathcal{E} should be chosen in such a way that the resulting densities do not depend on their precise values. In particular, E_{max} has to be larger than the absolute value of the depth of the potential well.

In the present version of the code we only consider single closed-shell nuclei, i.e. systems with spherical symmetry. The fields $\sigma(r)$, $\omega^0(r)$, $\rho^0(r)$, and $A^0(r)$ depend only on the radial coordinate r . The nucleon spinors U_k (V_k) in (2) are characterized by the angular momentum j , its z -projection m , parity π and the isospin $t_3 = \pm\frac{1}{2}$ for neutron and proton. We combine the two Dirac spinors $U_k(\mathbf{r})$ and $V_k(\mathbf{r})$ to form a *super-spinor*

$$\Phi_k(\mathbf{r}) := \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} \quad (22)$$

where

$$U_k(V_k)(\mathbf{r}, s, t_3) = \begin{pmatrix} g_{U(V)}(r)\Omega_{j,l,m}(\theta, \varphi, s) \\ if_{U(V)}(r)\Omega_{j,\tilde{l},m}(\theta, \varphi, s) \end{pmatrix} \chi_\tau(t_3). \quad (23)$$

$g(r)$ and $f(r)$ are radial amplitudes, χ_τ is the isospin function, the orbital angular momenta l and \tilde{l} are determined by j and the parity π

$$l = \begin{cases} j + 1/2 & \text{for } \pi = (-1)^{j+1/2} \\ j - 1/2 & \text{for } \pi = (-1)^{j-1/2} \end{cases}, \quad (24)$$

and

$$\tilde{l} = \begin{cases} j - 1/2 & \text{for } \pi = (-1)^{j+1/2} \\ j + 1/2 & \text{for } \pi = (-1)^{j-1/2} \end{cases} \quad (25)$$

Ω_{jlm} is the tensor product of the orbital and spin functions

$$\Omega_{j,l,m}(\theta, \varphi, s) = \sum_{m_s, m_l} \langle \frac{1}{2} m_s l m_l | j m \rangle \chi_{\frac{1}{2} m_s} Y_{lm_l}(\theta, \varphi). \quad (26)$$

It will be useful to define a single angular quantum number κ as the eigenvalue of the operator $(1 + \hat{\sigma} \cdot \hat{\mathbf{l}})$

$$(1 + \hat{\sigma} \cdot \hat{\mathbf{l}}) \Omega_{\kappa,m} = -\kappa \Omega_{\kappa,m}, \quad (27)$$

$$\kappa = \pm(j + 1/2) \quad \text{for } j = l \mp 1/2. \quad (28)$$

$\kappa = \pm 1, \pm 2, \pm 3, \dots$, and the Dirac HB equations are solved in coordinate space for each value of κ . The equations for the radial amplitudes $g_{U(V)}(r)$ and $f_{U(V)}(r)$ are derived from Eq. (2). The radial single-particle Dirac Hamiltonian reads (see also appendix A)

$$\hat{h}_\kappa(r) - m := \sigma_3 \sigma_1 (\partial_r + r^{-1}) - \sigma_1 \kappa r^{-1} + (\sigma_3 - \mathbf{1}_2) m + \sigma_3 S(r) + \mathbf{1}_2 V_0(r), \quad (29)$$

where the scalar and vector potentials are

$$S(r) = g_\sigma \sigma(r), \quad \text{and} \quad V^0(r) = g_\omega \omega^0(r) + g_\rho \tau_3 \rho_3^0(r) + e \frac{(1 - \tau_3)}{2} A^0(r). \quad (30)$$

σ_i (i=1,2,3) are the Pauli matrices. The integral operator of the pairing interaction takes the form

$$\hat{\Delta}(r) = \int_0^\infty dr' r'^2 \Delta(r, r') \quad (31)$$

The kernel of the integral operator is defined

$$\Delta_{aa'}^{JM}(r, r') = \frac{1}{2} \sum_{\tilde{a}, \tilde{a}'} \langle r a, r' a' | \hat{V} | r \tilde{a}, r' \tilde{a}' \rangle_{JM} \kappa_{\tilde{a}, \tilde{a}'}(r, r') \quad (32)$$

where r and r' denote radial coordinates, a, a', \tilde{a} and \tilde{a}' are quantum numbers that completely specify single-nucleon states: (n, l, j, m) or (n, κ, m) , J and M are the total angular momentum of the pair, and its z -projection, respectively. For the pairing interaction we use the finite range Gogny force

$$V^{pp}(1, 2) = \sum_{i=1,2} e^{-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{\mu_i^2}} (W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau). \quad (33)$$

We only consider contributions from $J = 0$ pairs to the pairing matrix elements. The kernel of the integral operator can then be written

$$\Delta_\kappa(r, r') = \frac{1}{2} \sum_{\tilde{\kappa}} V_{\kappa\tilde{\kappa}}^{J=0}(r, r') \kappa_{\tilde{\kappa}}(r, r'). \quad (34)$$

Details on the calculation of two-body matrix elements of the Gogny force are given in Appendix B. The pairing tensor is calculated

$$\kappa_\kappa(r, r') = \sum_n 2|\kappa| \begin{pmatrix} g_{n,\kappa}^{(U)}(r) g_{n,\kappa}^{(V)}(r') & 0 \\ 0 & f_{n,\kappa}^{(U)}(r) f_{n,\kappa}^{(V)}(r') \end{pmatrix} \quad (35)$$

where, for a quantum number κ , the sum runs over all solutions in the specified energy interval $0 < E < E_{\max}$. If we define $\Phi_{U(V)}(r) := (g_{U(V)}(r), f_{U(V)}(r))^T$, the radial Dirac-Hartree-Bogoliubov equations read

$$\begin{aligned} (\hat{h}_D(r) - m - \lambda) \Phi_U(r) + \int_0^\infty dr' r'^2 \Delta(r, r') \Phi_V(r') &= E \Phi_U(r) \\ (-\hat{h}_D(r) + m + \lambda) \Phi_V(r) + \int_0^\infty dr' r'^2 \Delta(r, r') \Phi_U(r') &= E \Phi_V(r) \end{aligned} \quad (36)$$

The meson and photon fields are solution of the Klein-Gordon equations

$$(-\partial_r^2 - \frac{2}{r} \partial_r + \frac{l(l+1)}{r^2} + m_\sigma^2) \sigma(r) = -g_\sigma \rho_s(r) - g_2 \sigma^2(r) - g_3 \sigma^3(r) \quad (37)$$

$$(-\partial_r^2 - \frac{2}{r} \partial_r + \frac{l(l+1)}{r^2} + m_\omega^2) \omega^0(r) = -g_\omega \rho_v(r) \quad (38)$$

$$(-\partial_r^2 - \frac{2}{r} \partial_r + \frac{l(l+1)}{r^2} + m_\rho^2) \rho^0(r) = -g_\rho \rho_3(r) \quad (39)$$

$$(-\partial_r^2 - \frac{2}{r} \partial_r + \frac{l(l+1)}{r^2}) A^0(r) = e \rho_p(r). \quad (40)$$

where $l = 0$ for spherical nuclei. In the following we describe the computer code used to solve the system of equations (36) to (40) in a self-consistent iteration scheme.

3 Finite Element discretization of the radial equations

The radial equations (36) - (40) can be written in the general form

$$\hat{H}(\lambda, r, \sigma(r), \omega^0(r), \rho^0(r), A^0(r), \Delta(r), \lambda) \Phi_i(r) = \varepsilon_i \Phi_i(r) \quad (41)$$

$$\hat{R}_\sigma(r, \sigma(r))\sigma(r) = s_\sigma(\Phi_1(r), \dots, \Phi_A(r)) \quad (42)$$

$$\hat{R}_\omega(r)\omega^0(r) = s_\omega(\Phi_1(r), \dots, \Phi_A(r)) \quad (43)$$

$$\hat{R}_\rho(r)\rho^0(r) = s_\rho(\Phi_1(r), \dots, \Phi_A(r)) \quad (44)$$

$$\hat{R}_C(r)A^0(r) = s_C(\Phi_1(r), \dots, \Phi_Z(r)). \quad (45)$$

where \hat{H} is a 4×4 matrix operator defined as

$$\hat{H} := \begin{pmatrix} S(r) + V(r) - \lambda & \partial_r - (\kappa_i - 1)r^{-1} & \hat{\Delta}^{(gg)}(r) & 0 \\ -\partial_r - (\kappa_i + 1)r^{-1} & -2m - S(r) + V(r) - \lambda & 0 & \hat{\Delta}^{(ff)}(r) \\ \hat{\Delta}^{(gg)}(r) & 0 & -S(r) - V(r) + \lambda & -\partial_r + (\kappa_i - 1)r^{-1} \\ 0 & \hat{\Delta}^{(ff)}(r) & \partial_r + (\kappa_i + 1)r^{-1} & 2m + S(r) - V(r) + \lambda \end{pmatrix}. \quad (46)$$

and

$$\hat{R}_\sigma := -\partial_r^2 - 2r^{-1}\partial_r + l(l+1)r^{-2} + m_\sigma^2 + g_2\sigma(r) + g_3\sigma^2(r) \quad (47)$$

$$\hat{R}_\omega := -\partial_r^2 - 2r^{-1}\partial_r + l(l+1)r^{-2} + m_\omega^2 \quad (48)$$

$$\hat{R}_\rho := -\partial_r^2 - 2r^{-1}\partial_r + l(l+1)r^{-2} + m_\rho^2 \quad (49)$$

$$\hat{R}_C := -\partial_r^2 - 2r^{-1}\partial_r + l(l+1)r^{-2}. \quad (50)$$

The source terms on the right hand sides of these equations are defined as $s_\sigma := -g_\sigma \rho_s(r)$, $s_\omega := g_\omega \rho_v(r)$, $s_\rho := g_\rho \rho_3(r)$, and $s_C := e \rho_{\text{em}}(r)$. The method of finite elements is used to discretize the system of Dirac-Hartree-Bogoliubov and Klein-Gordon equations on a spherical mesh. For the nucleon spinor we define $\Psi(r) := (\Phi_U(r)^T, \Phi_V(r)^T)^T$, and use the FEM ansatz

$$\Psi(r) = \sum_p X_p N_p(r) \quad (X_p \in \mathbf{R}^4), \quad (51)$$

where the coefficients X_p are four-component vectors, and $N_p(r)$ denotes Lagrange shape functions of arbitrary order [13]. The index p enumerates nodes on a finite element mesh for a spherical box ($r_{\min} = 0$ to r_{\max}). r_p denotes the radial coordinate of the node p . The Lagrange shape functions N_p satisfy the property $N_p(r_{p'}) = \delta_{pp'}$. Therefrom the coefficients X_p in the ansatz (51) correspond to the amplitudes $\Psi(r_p)$ of the solution: $X_p = (g^{(U)}(r_p), f^{(U)}(r_p), g^{(V)}(r_p), f^{(V)}(r_p))^T$. The Dirac-Hartree-Bogoliubov equations can be formally written

$$\hat{D}(\Psi) = f(\Psi, x) \quad (52)$$

where \hat{D} is a differential operator. For any approximate solution $\tilde{\Psi}(x)$, the residual error is defined as

$$R(x) := \hat{D}(\tilde{\Psi}) - f(\tilde{\Psi}, x). \quad (53)$$

If (52) has to be solved on a compact domain $\Omega \subset \mathbf{R}^n$, where $\Psi(x) = g(x)$ for $x \in \partial\Omega$, and $g(x)$ is defined on the boundary $\partial\Omega$ of Ω , the method of weighted residuals can be used to define the weak form of the boundary value problem

$$\int_{\Omega} R(x) w(x) d^n x \equiv 0 \quad \text{for all weight functions } w(x). \quad (54)$$

The method of weighted residuals necessitates that a weighted integral of the residual vanishes. In the Galerkin method the choice of weight functions is $w_p(x) \equiv N_p(x)$, where

$N_p(x)$ are shape functions that define the FEM ansatz of the solution. As we have shown in Ref. [13], the choice $w_p(r) = r^2 N_p(r)$ produces symmetric stiffness matrices for the radial equations. Using the standard representation for the Pauli matrices, the radial relativistic Hartree-Bogoliubov equations (36) can be written in matrix form

$$\begin{aligned} & \left[(\partial_r + r^{-1}) \sigma_3 \otimes \sigma_3 \sigma_1 - \kappa r^{-1} \sigma_3 \otimes \sigma_1 + m \sigma_3 \otimes (\sigma_3 - \mathbf{1}_2) + S(r) \sigma_3 \otimes \sigma_3 + \right. \\ & \left. V_0(r) \sigma_3 \otimes \mathbf{1}_2 + \sigma_1 \otimes \mathbf{1}_2 \hat{\Delta}(r) - \lambda \sigma_3 \otimes \mathbf{1}_2 \right] \Psi(r) - E \mathbf{1}_4 \Psi(r) = 0 \end{aligned} \quad (55)$$

Eq. (55) represents a system of four coupled integro-differential equations. For the matrices which define the structure of these equations we use the notation

$$\begin{aligned} \mathbf{A}_1 &:= \sigma_3 \otimes \sigma_3 \sigma_1, & \mathbf{A}_2 &:= \sigma_3 \otimes \sigma_1, & \mathbf{A}_3 &:= \sigma_3 \otimes (\sigma_3 - \mathbf{1}_2), \\ \mathbf{A}_4 &:= \sigma_3 \otimes \sigma_3, & \mathbf{A}_5 &:= \sigma_3 \otimes \mathbf{1}_2, & \mathbf{A}_6 &:= \sigma_1 \otimes \mathbf{1}_2; \end{aligned} \quad (56)$$

The method of weighted residuals transforms the Dirac-Hartree-Bogoliubov equations into a finite system of algebraic equations. The system forms a generalized eigenvalue problem $\mathbf{A} X = \varepsilon \mathbf{N} X$ with global stiffness matrices

$$\begin{aligned} \mathbf{A} = \langle w_{p'} | & (\partial_r + r^{-1}) \mathbf{A}_1 - \kappa r^{-1} \mathbf{A}_2 + m \mathbf{A}_3 - \lambda \mathbf{A}_5 + S(r) \mathbf{A}_4 + \\ & V_0(r) \mathbf{A}_5 + \mathbf{A}_6 \hat{\Delta}(r) | N_p \rangle \end{aligned} \quad (57)$$

and

$$\mathbf{N} = \langle w_{p'} | \mathbf{1}_4 | N_p \rangle. \quad (58)$$

The number of equations in the system is thus four times the number of nodes on the finite element mesh. The eigenvalue matrix equation reads

$$\begin{aligned} & \left[\mathbf{S}_1 \otimes \mathbf{A}_1 + \mathbf{S}_2 \otimes \mathbf{A}_1 - \kappa \mathbf{S}_2 \otimes \mathbf{A}_2 + m \mathbf{S}_3 \otimes \mathbf{A}_3 + \mathbf{S}_4 \otimes \mathbf{A}_4 + \mathbf{S}_5 \otimes \mathbf{A}_5 + \mathbf{S}_6 \otimes \mathbf{A}_6 - \lambda \mathbf{S}_3 \otimes \mathbf{A}_5 \right] x \\ & = \varepsilon \left[\mathbf{S}_3 \otimes \mathbf{1}_4 \right] x \end{aligned} \quad (59)$$

where x is a vector with components $(x_1^{(gU)}, x_1^{(fU)}, x_1^{(gV)}, x_1^{(fV)}, \dots, x_n^{(gU)}, x_n^{(fU)}, x_n^{(gV)}, x_n^{(fV)})^T$. The global stiffness matrices \mathbf{S}_1 to \mathbf{S}_6 correspond to the various operator terms in Eq. (55)

$$\begin{aligned} \mathbf{S}_1 &= \left[\langle w_{p'}(r) | \partial_r | N_p(r) \rangle \right], \\ \mathbf{S}_2 &= \left[\langle w_{p'}(r) | r^{-1} | N_p(r) \rangle \right], \\ \mathbf{S}_3 &= \left[\langle w_{p'}(r) | N_p(r) \rangle \right], \\ \mathbf{S}_4 &= \left[\langle w_{p'}(r) | S(r) | N_p(r) \rangle \right], \\ \mathbf{S}_5 &= \left[\langle w_{p'}(r) | V(r) | N_p(r) \rangle \right], \\ \mathbf{S}_6 &= \left[\langle w_{p'}(r') | \Delta(r', r) r^2 | N_p(r) \rangle \right]. \end{aligned} \quad (60)$$

Details of the calculation and construction of the matrices \mathbf{S}_1 to \mathbf{S}_5 have been described in Appendix A of Ref. [13]. The matrix elements of \mathbf{S}_6 have to be calculated for the nonlocal

pairing interaction $\Delta(r', r)$. Using the same notation as in Ref. [13], the matrix elements of the local stiffness matrix in the reference element representation are

$$\begin{aligned} \mathbf{S}_6^{\text{loc}} &= \left[\langle N_{q'} | r'^2 \Delta(r', r) r^2 | N_q \rangle \right] = \\ &= \left[m^2 \Delta \zeta^2 a^6 \int_0^1 d\rho' \int_0^1 d\rho N_{q'}(\rho') (\zeta_{p'} + \Delta \zeta \rho')^{3m-1} \right. \\ &\quad \left. \Delta(a(\zeta_{p'} + \Delta \zeta \rho')^m, a(\zeta_p + \Delta \zeta \rho)^m) (\zeta_p + \Delta \zeta \rho)^{3m-1} N_q(\rho) \right] \end{aligned} \quad (61)$$

For the FEM discretization of the Klein-Gordon equations we use the ansatz

$$\sigma(r) = \sum_p \sigma_p N_p(r) \quad (62)$$

$$\omega^0(r) = \sum_p \omega_p^0 N_p(r) \quad (63)$$

$$\rho^0(r) = \sum_p \rho_p^0 N_p(r) \quad (64)$$

$$A^0(r) = \sum_p A_p^0 N_p(r). \quad (65)$$

where the node variables σ_p , ω_p^0 , ρ_p^0 and A_p^0 correspond to field amplitudes at the mesh point p. For the Klein-Gordon equations we use the same type of shape functions $N_p(r)$, and the same mesh as in the FEM discretization of the RHB equation (55). In this way we obtain the following algebraic equations for the mean field amplitudes of the meson fields

$$\left[S_1^\sigma + l(l+1) S_2^\sigma + m_\sigma^2 S_3^\sigma + S_4^\sigma \right] \vec{\sigma} = \vec{r}^{(s)} \quad (66)$$

$$\left[S_1^\omega + l(l+1) S_2^\omega + m_\omega^2 S_3^\omega \right] \vec{\omega}^0 = \vec{r}^{(v)} \quad (67)$$

$$\left[S_1^\rho + l(l+1) S_2^\rho + m_\rho^2 S_3^\rho \right] \vec{\rho}^0 = \vec{r}^{(3)} \quad (68)$$

$$\left[S_1^{A^0} + l(l+1) S_2^{A^0} \right] \vec{A}^0 = \vec{r}^{(\text{em})}. \quad (69)$$

The node variables σ_p , ω_p^0 , ρ_p^0 and A_p^0 are grouped into the vectors $\vec{\sigma} = (\sigma_1, \dots, \sigma_n)^T$, $\vec{\omega}^0 = (\omega_1, \dots, \omega_n)^T$, $\vec{\rho}^0 = (\rho_1^0, \dots, \rho_n^0)^T$, $\vec{A}^0 = (A_1^0, \dots, A_n^0)^T$, and

$$S_1^\sigma = S_1^\omega = S_1^\rho = S_1^A = \langle w_{p'}(r) | \partial_r^2 + 2r^{-1} \partial_r | N_p(r) \rangle, \quad (70)$$

$$S_2^\sigma = S_2^\omega = S_2^\rho = S_2^A = \langle w_{p'}(r) | r^{-2} | N_p(r) \rangle, \quad (71)$$

$$S_3^\sigma = S_3^\omega = S_3^\rho = S_3^A = \langle w_{p'}(r) | N_p(r) \rangle, \quad (72)$$

$$S_4^\sigma = \langle w_{p'}(r) | g_2 \sigma(r) + g_3 \sigma(r)^2 | N_p(r) \rangle. \quad (73)$$

The components of the right hand side vectors are defined as

$$\begin{aligned} r_{p'}^{(s)} &= -g_\sigma \langle w_{p'}(r) | \rho_s(r) \rangle, \\ r_{p'}^{(v)} &= g_\omega \langle w_{p'}(r) | \rho_v(r) \rangle, \\ r_{p'}^{(3)} &= g_\rho \langle w_{p'}(r) | \rho_3(r) \rangle, \\ r_{p'}^{(\text{em})} &= e \langle w_{p'}(r) | \rho_{\text{em}}(r) \rangle. \end{aligned} \quad (74)$$

Details on the calculation of the stiffness matrices $\mathbf{S}_1^\sigma, \mathbf{S}_2^\sigma, \mathbf{S}_3^\sigma, \mathbf{S}_4^\sigma, \mathbf{S}_1^\omega, \mathbf{S}_2^\omega, \mathbf{S}_3^\omega, \mathbf{S}_1^\rho, \mathbf{S}_2^\rho, \mathbf{S}_3^\rho, \mathbf{S}_1^{A^0}, \mathbf{S}_2^{A^0}$, and the right-hand side vectors $\vec{r}^{(s)}, \vec{r}^{(v)}, \vec{r}^{(3)}, \vec{r}^{(\text{em})}$, are given in Appendix B of Ref. [13]. Next we discuss the structure and occupation pattern of the global stiffness matrices of the RHB equation and describe the inclusion of boundary conditions. The boundary conditions for the spherical symmetric case are

$$\begin{aligned} f^{(U)}(r=0) &= 0 \quad \text{and} \quad f^{(V)}(r=0) = 0 \quad \text{for} \quad \kappa = -1 \\ g^{(U)}(r=0) &= 0 \quad \text{and} \quad g^{(V)}(r=0) = 0 \quad \text{for} \quad \kappa = +1 \\ g^{(U)}(r=0) &= 0 \quad \text{and} \quad f^{(U)}(r=0) = 0 \quad \text{for} \quad |\kappa| > 1 \\ g^{(V)}(r=0) &= 0 \quad \text{and} \quad f^{(V)}(r=0) = 0 \quad \text{for} \quad |\kappa| > 1 \end{aligned} \quad (75)$$

and

$$g^{(U)}(r_{\text{max}}) = 0 \quad \text{and} \quad g^{(V)}(r_{\text{max}}) = 0 \quad \text{for all} \quad \kappa. \quad (76)$$

In Figs. 3 (a) and (b) we display the occupation pattern of the global stiffness matrices A and N , respectively. The occupation pattern corresponds to first order finite elements (linear shape functions). Shaded squares indicate the positions of non-zero matrix elements. The occupation pattern displays a dominant block diagonal band structure. This structure results from the contributions of the local terms in (55). Each diagonal block consists of several 4×4 -blocks. The number of 4×4 -blocks is determined by the order of finite elements: $(n_{\text{ord}} + 1)^2$. From Eq.(59) we notice that the occupation pattern in a 4×4 -block results from a superposition of occupation patterns of the matrices A_k (56). Non-zero matrix elements outside the block diagonal band structure result from nonlocal terms that correspond to the finite range pairing interaction (dark shaded squares in Fig. 3 (a)). In the Figs. 3 (c) and (d), and Figs. 3 (e) and (f) we display the occupation patterns for the choice of second and third order finite elements, respectively. To each pair of nodes (p, p') on the finite element mesh, there corresponds a 4×4 -block $\langle w_p | \hat{H} | N_{p'} \rangle$, which has to be multiplied by a vector $X_{p'}$. Depending on the boundary conditions (75), one or more components of $X_{p'}$ are set to zero. Boundary conditions are taken into account by simply eliminating columns and rows with the corresponding index from both stiffness matrices \mathbf{A} and \mathbf{N} . We illustrate this procedure in Figs. 3 (a) and (b) for the case $\kappa = -1$ (boundaries $r = 0$ and $r = r_{\text{max}}$). In the Figs. 3 (c) and (d) the boundary conditions correspond to $\kappa = +1$, while in the Figs. 3 (e) and (f) boundary conditions for the case $|\kappa| > 1$ are displayed.

4 An illustrative calculation

In this section we present an illustrative calculation for the ground state of the spherical nucleus ^{124}Sn . The self-consistent calculation is performed for the mean-field parameter set NL1[17], and the D1S [19] parameters for the finite range pairing interaction (33). The $Z = 50$ protons in Sn form a closed shell. Single-particle wave functions of proton states are calculated as solutions of the radial Dirac equation, as described in Ref. [13]. $N = 74$ neutrons in the isotope ^{124}Sn partially occupy the major shell $N = 50 - 82$. For neutrons we solve the radial RHB-equations (36), and Klein-Gordon equations (37) to (40) for the meson and photon fields. In the initial step of the self-consistent iteration, Woods-Saxon shapes are used

$$S(r) = S(0) \left(1 + \exp \left(\frac{r - r_s}{a} \right) \right)^{-1}, \quad (77)$$

$$V(r) = V(0) \left(1 + \exp \left(\frac{r - r_s}{a} \right) \right)^{-1}. \quad (78)$$

for the scalar σ and vector ω potentials. The contribution of the ρ -meson to the effective potential is set to zero in the first iteration step. The initial Coulomb potential corresponds to a homogenous spherical charge distribution of radius r_s . For ^{124}Sn the initial values of the scalar and vector potentials at $r = 0$ are chosen $S(0) = -395 \text{ MeV}$ and $V(0) = 320 \text{ MeV}$, respectively. $a = 0.5 \text{ fm}$ and $r_s = 6.0 \text{ fm}$. The RHB equations are solved for $\kappa = \pm 1, \dots, \pm 7$. The inclusion of additional κ -blocks in the self-consistent calculation did not change the results for ground state properties. As is illustrated in the energy diagram in Fig. 2, the diagonalization of the resulting eigenvalue problem is performed in a window of positive quasi-particle energies $[0, 100] \text{ MeV}$.

In each step of the self-consistent iteration, the value of the chemical potential λ has to be adjusted in such a way that the expectation value of the particle number operator equals the number of neutrons, i.e. 74 in this case. The correct value of λ is found as the root of the function

$$dn(\lambda) := N - \sum_{\kappa} \sum_n \int_0^{\infty} dr r^2 (g_{n,\kappa}^{(V)}(\lambda, r)^2 + f_{n,\kappa}^{(V)}(\lambda, r)^2) \quad (79)$$

where N is the number of neutrons, and the second term is the trace of the density matrix. In the initial steps of the self-consistent iteration, λ is not calculated with a very high precision. The precision increases with the number of iteration steps, i.e. with the accuracy with which the mean-field is calculated. If $\lambda_0^{(i)}$ is the calculated value of the chemical potential in the i -th iteration step, we define an interval $I^{(i+1)} := [\lambda_0^{(i)} - \Delta\lambda^{(i)}, \lambda_0^{(i)} + \Delta\lambda^{(i)}]$ in which the new value $\lambda_0^{(i+1)}$ is to be found. The width of the interval is defined

$$\Delta\lambda^{(i)} = \frac{\Delta\lambda^{(0)}}{(i+1)^n} \quad (80)$$

where $\Delta\lambda^{(0)}$ is an input parameter, and we take $n = 2$. This procedure leads to good convergence, and accurate values of λ are obtained when the iterations approach the self-consistent solution. After the first few RHB iterations, the number of nested λ -iteration steps varies between 1 and 3.

In what follows we present results for the self-consistent solution that correspond to the ground state of ^{124}Sn . The meson fields have been calculated with precision 10^{-3} MeV , and the accuracy for single quasi-particle energies is 10^{-4} MeV . In Figs. 4a, 4b, 4c, and 4d we display the normalized amplitudes of the quasi-particle spinors. The normalization for quasi-particle states is defined:

$$1 = \int d^3r (\Phi_U^\dagger(\mathbf{r})\Phi_U(\mathbf{r}) + \Phi_V^\dagger(\mathbf{r})\Phi_V(\mathbf{r})) \quad (81)$$

In Fig. 5 we display the baryon densities (8) calculated with 150 linear shape functions in a radial box of 30 fm. The dashed curve corresponds to the density calculated in the first iteration step with the initial Woods-Saxon potentials, and the solid curve is the self-consistent result. Since the densities are very sensitive to the details of the numerical approximations, we use them to choose the most effective cut-off in the stiffness matrices of the Hartree-Bogoliubov equations. Namely, as explained in Section 5, we only construct stiffness matrices with band diagonal structure. The width of the bands is an

input parameter, i.e. the cut-off parameter of the matrices. A too small value of the cut-off parameter means that many off-diagonal matrix elements of the pairing interaction are neglected. A large cut-off makes the diagonalization of the algebraic eigenvalue equations slow. In the calculation of the baryon density in Fig. 5 we have used a cut-off value of 50. The resulting global stiffness matrices have a band diagonal structure of width 101. This value is too small, and unphysical oscillations of the density are observed. The amplitude of these oscillations corresponds to the values of the largest pairing matrix elements that have been neglected. Most of our calculations, and in particular the results that follow, have been performed with a cut-off parameter 60.

In Fig. 6 we show, for each value of the κ -quantum number, the contributions of individual quasi-particle states to the pairing field. We plot the quantities

$$\begin{pmatrix} \Delta_V^{(g)}(r) \\ \Delta_V^{(f)}(r) \end{pmatrix} = \int_0^{r_{max}} dr' r'^2 \begin{pmatrix} \Delta^{(gg)}(r, r') & 0 \\ 0 & \Delta^{(ff)}(r, r') \end{pmatrix} \begin{pmatrix} g_{n\kappa}^{(V)}(r') \\ f_{n\kappa}^{(V)}(r') \end{pmatrix}. \quad (82)$$

The contributions to the pairing field are mainly concentrated on the the surface of the nucleus. In Fig. 7 we also display the integrated kernel of the integral operator of the pairing interaction

$$\begin{pmatrix} \Delta^{(g)}(r) \\ \Delta^{(f)}(r) \end{pmatrix} = \int_0^{r_{max}} dr' r'^2 \begin{pmatrix} \Delta^{(gg)}(r, r') & 0 \\ 0 & \Delta^{(ff)}(r, r') \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (83)$$

In order to illustrate how the single-particle density and pair matrices depend on the size r_{max} of the spherical box, in Fig. 8 we display the quantities $N_{n\kappa}$ and $P_{n\kappa}$ [5]

$$N_{n\kappa} = \int_0^{max} dr r^2 (g_{n\kappa}^{(V)}(r) g_{n\kappa}^{(V)}(r) + f_{n\kappa}^{(V)}(r) f_{n\kappa}^{(V)}(r)), \quad (84)$$

$$P_{n\kappa} = - \int_0^{max} dr r^2 (g_{n\kappa}^{(U)}(r) g_{n\kappa}^{(V)}(r) + f_{n\kappa}^{(U)}(r) f_{n\kappa}^{(V)}(r)), \quad (85)$$

which constitute a measure of the contribution of the n -th quasi-particle state to the density matrix ρ and to the pairing tensor κ , respectively. $(2j+1)N_n$ is the contribution to the particle number. In Figs. 8a and 8b we plot N_n and P_n as functions of quasi-particle energy for the $s_{1/2}$ -states ($\kappa = -1$). Self-consistent results are shown for three sizes of the radial box: $r_{max} = 15, 30$ and 40 fm. The precision of the calculations is: 10^{-3} MeV for the meson fields, and 10^{-4} MeV for the quasi-particle energies. The largest contributions to the density ρ come from the three quasi-particle states at 1.52 MeV, 26.18 MeV and 51.82 MeV). The state at 1.52 MeV, which is closest to the Fermi level λ , gives the largest contribution to the pairing tensor. For $\kappa = -1$ the contribution to the pairing comes from these three peaks that represent bound states. Both quantities, N_n and P_n , asymptotically decay with increasing quasi-particle energy. Therefore, an extension of the energy window above 100 MeV would not change the calculated quantities. Similar results are obtained for other values of κ . In Tables 1 and 2 we illustrate the numerical accuracy with which calculations can be performed. From 80 to 200 linear finite elements have been used in the calculations. 14 values of κ are included: $\kappa = -7$ to $\kappa = +7$. In Table 1 quantities that characterize the bulk properties of ^{124}Sn are displayed. For all quantities we observe convergence with the increase of the size of the radial box, and of the quasi-particle energy

window. In addition, in the right column, we list the corresponding values calculated with a computer program that uses an expansion in oscillator basis functions [6]. For a nucleus that is still far away from the drip line, the finite element discretization and the oscillator basis expansion should produce very similar results. For drip line nuclei we expect the finite element method to provide more accurate solutions. r_{\max} and E_{\max} denote the size of the radial box and of the energy window, respectively. The energies \mathbf{E}_p and \mathbf{E}_n are defined as

$$\mathbf{E}_{n(p)} = \sum_i 2|\kappa_i|v_{i,n(p)}^2 E_{i,n(p)}, \quad (86)$$

where the $E_{i,n(p)}$ denotes the canonical energies, and $v_{i,n(p)}$ the occupation probabilities. The pairing field $\Delta_{aa}(r, r')$ and the pairing tensor $\kappa_{aa}(r, r')$ are used to calculate the pairing energy \mathbf{E}_{pair}

$$E_{\text{pair}} = \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 \sum_a \kappa_{aa}(r, r') \Delta_{aa}(r, r'). \quad (87)$$

The sum in (87) runs over all values of κ . In addition we display in Table 1 the total energy of the σ -field \mathbf{E}_{sig} , the contribution of nonlinear terms to the σ -energy \mathbf{E}_{nl} , the energy of the ω -field \mathbf{E}_{ome} , the energy of the ρ -field \mathbf{E}_{rho} , the Coulomb energy \mathbf{E}_{pho} , the total binding energy \mathbf{E}_b and the binding energy per nucleon $\frac{\mathbf{E}_b}{A}$. These quantities are defined in Refs. [13] and [22]. The mean square radii \mathbf{rms} are defined

$$\mathbf{rms} = \sqrt{\frac{\int_0^\infty dr r^4 \sum_i 2|\kappa_i| \Phi_{V,i}^\dagger(r) \Phi_{V,i}(r)}{\int_0^\infty dr r^2 \sum_i 2|\kappa_i| \Phi_{V,i}^\dagger(r) \Phi_{V,i}(r)}} \quad (88)$$

In Table 2 we compare results for canonical energies and occupation probabilities of single-neutron states in ^{124}Sn .

5 Program structure

The program is coded in C++. The implementation of the relativistic mean field model in the Hartree approximation for spherical doubly-closed shell nuclei has been described in Ref. [13]. In this section we only describe the changes that have been made in order to extend the program to open-shell nuclei, and include pairing correlations in the framework of relativistic Hartree-Bogoliubov theory.

The main part of the program consists of seven classes: **MathPar**: numerical parameters used in the code, **PhysPar**: physical parameters (masses, coupling constants, etc.), **FinEl**: finite elements, **Mesh**: mesh in coordinate space, **Nucleon**: neutrons and protons in the nuclear system, **Meson**: mesons and photon with corresponding mean fields and the Coulomb field, and the class **LinBCGOp**. A detailed description of these classes can be found in Ref. [13]. In the following we describe additional methods and parameters that are used in the present version of the program. The program allows one type of nucleons (protons or neutrons) to partially occupy a major shell of the nuclear shell model. A partially occupied major shell is referred to as an open shell. Nuclei with both proton and neutron shells open are generally deformed. The program is restricted

to nuclear systems with spherical symmetry. For the type of nucleons that occupy open shells the relativistic Hartree Bogoliubov (RHB) equations have to be solved for a set of κ -quantum numbers: $\pm 1, \pm 2, \pm 3, \dots$. The class **MathPar** contains the new parameter *Kapa_max* which equals the maximal absolute value of κ . Other new parameters are: *Mesh_rmax_mes* for the size of the mesh on which the meson field equations are solved, *Nucleon_maxrhbst*[*PhysPar::NumNucTypes*] for the maximal number of quasi-particle states, *Lambda0* for the initial value of the chemical potential, *D_Lamb0* for the initial step in the λ -iteration procedure, and *Numb_rhb_tol* for the initial tolerance in the calculation of the number of particles for a particular value of λ . Due to nonconservation of the number of particles, solutions of RHB equations in general do not correspond to the correct number of nucleons. In the λ -iteration the value of the chemical potential is adjusted in such a way that the expectation value of the particle number operator (trace of the density matrix), equals the number of nucleons for the specific nucleus.

The set of physical parameters of the nucleus, contained in the class **PhysPar**, is extended by the parameter *RHB_nuc_number*[*PhysPar::NumNucTypes*], which is the number of nucleons for which the RHB equations are solved. The prototype method *set_nucleus_XX()* can be used to define the numbers of protons and neutrons. In addition to the mean field parameter sets NL1, NL2, NLSH and NL3, the class **PhysPar** contains two parameter sets for the Gogny interaction: D1 [18] and D1S [19].

Essential changes have been made in the class **nucleon**. The method *solve(Meson const& _sigma, Meson const& _omega, Meson const& _rho, Meson const& _photon)* distinguishes between nucleons that occupy closed shells, for which the Dirac equation has to be solved, and nucleons in open shells, for which the wave functions are solutions of Hartree-Bogoliubov equations. A new constructor *make_gog_stiff(int nvec,int ikap,int *iab,int *iz,double* A,double *N)* for stiffness matrices of the RHB equations has been added to the class. *make_gog_stiff* is used only in the first step of the λ -iteration, for each κ . The method *store_gog_stiff(int nvec,int ndx,int ikap,int* iab,int* iz, double* A, double *N)* stores the resulting stiffness matrices in the private fields *int**siz*, *int**siab*, *double**SA*, and *double**SB*. If the diagonalization has to be repeated just for a different value of the chemical potential, the reconstruction of the stiffness matrices is performed by *read_gog_stiff(nvec,ndx,ikap,iab,iz,A,N)* and *make_new_lamb_gog_stiff(A,lamb,lamb_old)*. Matrix elements that depend on λ are replaced with new values. *boucond(kapa,nvec,n_eig,iab,iz,A,N,&nvec2,&n2)* includes boundary conditions in the stiffness matrices. Rows and columns are eliminated, and the resulting matrices are written in condensed form.

The largest matrix elements of the finite range pairing interaction are concentrated near the diagonal of the stiffness matrix. The absolute values of the pairing matrix elements monotonically decrease as one goes away from the diagonal, and the outermost are many orders of magnitude smaller than those at the diagonal. Therefore, elements of the stiffness matrices are only calculated in blocks within a band diagonal structure. The *mat_cutoff(int nvec2,int n2,int* iz,int* iab,double *A,double* N, int* nvec3,int* ndf3)* removes from the global stiffness matrix all elements which lie outside a band of chosen width, and performs a condensation of the matrix. The eigenvalue problem with band matrix structure is solved by the bisection method *bisec(n2,A,N,iab,iz,en_low_rhb,en_upper_rhb,tol,lam,XX,ndx,mdx,ndf3)*. Eigenvalues and eigenvectors are calculated in a window [*low_rhb*; *upper_rhb*] of the energy parameter.

The function *elim_spur_rhb(mdx,XX,lam,ist,&numb_lev,kapa)* eliminates spurious solutions from the spectrum produced by *bisec*. *add_dens_rhb* adds contributions to the source

terms of the boson fields. For a calculation performed with some value of the chemical potential, the method *trace_dens(int ist,int numb_lev,int kapa)* calculates the trace of the density matrix for each κ . A combination of the secant method and the bisection method is used by *calc_new_lambda_secant(lamb_iter,dn,&la_l,&la_r,&dn_l,&dn_r, lam_old)* to calculate new λ values. In the following table we list all the new member functions which have been included in the class **nucleon**.

List of new member functions in class nucleon:

```
void write_canon_energies( double** vv, double** Ec );
void write_solutions(int kapa,double *lam,double **XX,int mdx );
void write_rhb_states(int k);
void write_canonical_basis(int kapa,int n,double **CG,double **CF);
void write_dens_kap(int k);
void write_stiff_matels(int k,int nvec,int n,int *iz,int *iab, double *A,double *B);
void calc_canonical_basis();
void calc_NnPn();
void scan_delta_wave(int k);
void scan_delta();
double energy_pair();
double energy_pair_delta();
double radius_ms();
double sum_r2();
double norm();
double fac(double n);
void make_kapa_list();
double guvwave( double const* g, int kapa, int ife, int iga ) const;
double fuvwave( double const* f, int kapa, int ife, int iga ) const;
void make_stiff_delta_force(int lamb_iter,int nvec,int ikap, int *iab,int *iz, double *ast,double *bst);
void make_gog_stiff(int nvec,int k,int *iab,int *iz, double *ast,double *bst);
void make_new_lamb_gog_stiff(double *ast,double lamb_new, double lamb_old);
void store_gog_stiff(int nvec,int n,int ikap,int *iab,int *iz, double *A,double *B);
void read_gog_stiff(int nvec,int n,int ikap,int *iab,int *iz, double *A,double *B);
void boucond(int kapa,int nvec,int n,int *iab,int *iz, double *ast,double *bst,int *nvec2,int *n2);
void mat_cutoff(int nvec,int n,int *iz,int *iab, double *ast,double *bst,int *nvec3,int *ndf3);

void calc_gofac();
void make_s3_locst( int ife, double** s3 );
void make_loc_gog_st(int ikap,int ife1,int ife2,double** s6, double** s7);
void make_loc_stiff_delta(int ikap,int ife1,double **s6, double** s7);
double delta(int swgf,int k1,int ife1,int iga1,int ife2,int iga2);
double delta_delt(int swgf,int k1,int ife1,int iga1);
void elim_spur_rhb(int mdx,double** XX,double const* lam, int ist,int *numb_lev,int kapa );
void pickup_rhb_state(int iw,int kapa,double const* X,double lam);
```

```

void setup_stiffmats();
void copy_new_old();
void calc_dens0_rhb();
double density_rhb(int ife,int iga);
void make_dens_matr(double *A,double *B,int *iab,int *iz, int cutoff,int *nvec,int *nn);
void make_kk_dens_matr(int k,double *A,double *B,int *iab,int *iz, int *nvec,int *n);
void make_dens_matr_sdiag(int k,double **A,int *n);
void add_dens_rhb(int ist,int numb_lev,int kapa);
void large_r_dens(double r_cutoff);
void bisec_lambda(int lamb_iter,double dn, double *la_l,double *la_r, double *dn_l,double
*dn_r);
void bisec_lambda(int lamb_iter,double dn,double *dn1,double *dn2);
void calc_new_lambda_BCS();
void calc_new_lambda_secant(int lamb_iter,double dn, double *la_l,double *la_r, double
*dn_l,double *dn_r, double *lam_old);
double calc_nfe_mes();
double pair_tens_kap(int swgf,int k,int ife1,int iga1, int ife2,int iga2);
double trace_dens(int ist,int numb_lev,int kapa);
double delta_lambda(double dn,double sum);
double add_sum(int ist,int numb_lev,int kapa);
double gofac0(double l1,double l2,double j1,double j2,double lam);
double gofac1(double l1,double l2,double j1,double j2,double lam);
double pl(int l, double x);
double vl(int l,int ife1,int iga1,int ife2,int iga2,double mu_gog);
double clebsh_gordon_coeff(double j1,double m1, double j2,double m2, double j3,double
m3);
double wig_3j(double j1, double j2, double j3, double m1, double m2, double m3);
double wig_6j(double j1, double j2, double j3, double l1, double l2, double l3);
double del(double j1, double j2, double j3);

```

For the meson fields there is a possibility to choose the size of the finite element mesh different from that used in the solution of the Hartree-Bogoliubov equations. In some cases we have found that, by taking a smaller radial box for the meson fields, better numerical accuracy is obtained for quasi-particle spinors that correspond to nucleon states in the continuum. The number of finite elements in the meson mesh is determined by the member function *double Meson::calc_nfe_mes()* in the constructor of the class **meson**. The size parameter of the radial box *r_max_mes* has been included in the class **mesh**. In *numutils.cc* we have included a new solver for matrix diagonalization *void sdiag(int n, double **a, double *d, double **x, double *e, int is)*. It is based on the Householder algorithm, and is used for matrices of dimension smaller than 1000×1000 . *sdiag* diagonalizes the extremely ill conditioned density matrices $\rho_{kk'}$ in the member function *calc_canonical_basis* of class **nucleon**. The diagonalization is performed in the final transformation of single quasi-particle solutions to the canonical basis of single particle states.

A RHB equations for nuclear systems with spherical symmetry

The coordinate transformation

$$\begin{aligned} \mathcal{T} : [0, \infty) \otimes [0, \pi) \otimes [0, 2\pi) &\longrightarrow \mathbf{R}^3 \\ (r, \theta, \phi) &\longmapsto (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta) \end{aligned} \quad (89)$$

defines the RHB equation (2) in spherical coordinates (r, θ, ϕ) .

$$\hat{H}_D = -i(\alpha_3 \partial_r + \alpha_1 \frac{1}{r} \partial_\theta + \alpha_2 \frac{1}{r \sin \theta} \partial_\phi) + V(r) + m \beta + S(r) \beta \quad (90)$$

is the Dirac hamiltonian in spherical coordinates. The standard representation is used for the matrices α_i ($i = 1, 2, 3$): $\alpha_i = \sigma_1 \otimes \sigma_i$, where σ_i are the Pauli matrices. For a system with spherical symmetry, the scalar and the vector potential read

$$\begin{aligned} \hat{S}(r) &= g_\sigma \sigma(r) \\ \hat{V}(r) &= g_\omega \omega^0(r) + g_\rho \vec{\tau} \vec{\rho}(\vec{r}) + e \frac{(1 - \tau_3)}{2} A^0(r) \end{aligned} \quad (91)$$

Single-particle eigenfunctions of the Dirac hamiltonian \hat{H}_D are at the same time eigenvectors of the total angular momentum \hat{J} , its z-component \hat{J}_z , and of the operator

$$\hat{K} := -i\beta(\Sigma_2 \partial_\theta - \frac{1}{\sin \theta} \Sigma_1 \partial_\phi), \quad (92)$$

where $\Sigma_i := \mathbf{1}_2 \otimes \sigma_i$ ($i = 1, 2, 3$). For the eigenfunctions of \hat{H}_D

$$\hat{K} \Psi_\kappa = -\kappa \Psi_\kappa \quad (\kappa = \pm 1, \pm 2, \pm 3, \dots), \quad (93)$$

and this relation motivates the ansatz

$$\Psi_{n,\kappa,m}^T(r, \theta, \phi) := (g_{n\kappa}(r), i f_{n,-\kappa}(r))^T \otimes (\Omega_{\kappa,m}(\theta, \phi), \Omega_{-\kappa,m}(\theta, \phi))^T. \quad (94)$$

The Dirac hamiltonian takes the form

$$\hat{H}_D = -i(\alpha_3 \partial_r + \gamma_3 r^{-1} \hat{K}) + \hat{V}(r) + m(\beta - \mathbf{1}_4) + \hat{S}(r) \beta, \quad (95)$$

and the left hand side operator of the RHB equation (2) for a spherical symmetric system reads

$$\hat{H}_{RHB} = \sigma_3 \otimes [-i(\alpha_3 \partial_r + \gamma_3 \frac{1}{r} \hat{K}) + \hat{V}(r) + m\beta + \hat{S}(r)\beta] - \lambda \sigma_3 \otimes \mathbf{1}_4 + \sigma_1 \otimes \hat{\Delta}(r). \quad (96)$$

The ansatz for the nucleon spinor in (2) is

$$\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} g^{(U)}(r) \Omega_{\kappa,m}(\theta, \phi) \\ i f^{(U)}(r) \Omega_{-\kappa,m}(\theta, \phi) \\ g^{(V)}(r) \Omega_{\kappa,m}(\theta, \phi) \\ i f^{(V)}(r) \Omega_{-\kappa,m}(\theta, \phi) \end{pmatrix} \quad (97)$$

where the radial functions $g(r)$ and $f(r)$ depend on the principal quantum number n , and on κ . The pairing tensor is defined $\kappa_{cd}(\vec{r}, \vec{r}') := U_c^*(\vec{r})V_d^T(\vec{r}')$, and we postulate

$$\kappa_{nn'\tilde{\kappa}\tilde{\kappa}'mm'}(r, r', \theta, \theta', \phi, \phi') = \begin{pmatrix} g_{n\tilde{\kappa}}^{(U)}(r)g_{n'\tilde{\kappa}'}^{(V)}(r')\Omega_{\tilde{\kappa}\tilde{m}}^*(\theta, \phi)\Omega_{\tilde{\kappa}'\tilde{m}'}^T(\theta', \phi') & 0 \\ 0 & f_{n\tilde{\kappa}}^{(U)}(r)f_{n'\tilde{\kappa}'}^{(V)}(r')\Omega_{-\tilde{\kappa}\tilde{m}}^*(\theta, \phi)\Omega_{-\tilde{\kappa}'\tilde{m}'}^T(\theta', \phi') \end{pmatrix}. \quad (98)$$

For a pairing interaction of finite range, the kernel $\Delta_{ab}(\mathbf{r}, \mathbf{r}')$ (11,) is written in the form

$$\Delta_{\kappa\kappa'}(r, \theta, \phi, r', \theta', \phi') = \frac{1}{2} \sum_{\tilde{n}, \tilde{n}'} \sum_{\tilde{\kappa}, \tilde{\kappa}'} \sum_{\tilde{m}, \tilde{m}'} V_{\kappa\kappa'\tilde{\kappa}\tilde{\kappa}'}(r, r') \delta_{\tilde{n}, \tilde{n}'} \delta_{\tilde{\kappa}\tilde{\kappa}'} \delta_{\tilde{m}\tilde{m}'} \kappa_{\tilde{n}\tilde{n}'\tilde{\kappa}\tilde{\kappa}'\tilde{m}\tilde{m}'}(r, r', \theta, \theta', \phi, \phi'), \quad (99)$$

and the integral operator (13) of the pairing field, as a function of spherical coordinates

$$\hat{\Delta}(r, \theta, \phi) = \int_0^\infty \int_0^\pi \int_0^{2\pi} dr' r'^2 d\theta' \sin \theta' d\phi' \frac{1}{2} \sum_{\tilde{\kappa}} V_{\kappa\kappa\tilde{\kappa}\tilde{\kappa}} \kappa_{\tilde{\kappa}\tilde{\kappa}}(r, \theta, \phi, r', \theta', \phi'). \quad (100)$$

B Two-nucleon matrix elements of the Gogny interaction

For isospin T=1 pairing, i.e. pairing interaction between identical nucleons, the Gogny force (33) can be written in the form

$$V(1, 2) = \sum_{i=1,2} V_i(|\mathbf{r}_1 - \mathbf{r}_2|) (A_i + B_i P^\sigma) \quad (101)$$

where the spin operator acting on the two-nucleon state is defined

$$P^\sigma |(\frac{1}{2} \frac{1}{2}) S\rangle = (2S - 1) |(\frac{1}{2} \frac{1}{2}) S\rangle = \begin{cases} +1 & \text{for } S = 1; \\ -1 & \text{for } S = 0; \end{cases} \quad (102)$$

The radial interaction

$$V_i(|\mathbf{r}_1 - \mathbf{r}_2|) = e^{-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{\mu_i^2}} \quad (103)$$

can be written as an infinite sum of terms, each separable in the angular coordinates of the two nucleons

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) = \sum_{\lambda=0}^{\infty} V_\lambda(r_1, r_2) P_\lambda(\cos \theta_{12}), \quad (104)$$

where

$$P_\lambda(\cos \theta_{12}) = \frac{4\pi}{2\lambda + 1} \sum_{\mu} Y_{\lambda\mu}^*(\hat{\mathbf{r}}_1) Y_{\lambda\mu}(\hat{\mathbf{r}}_2), \quad (105)$$

and

$$V_\lambda(r_1, r_2) = \frac{2\lambda + 1}{2} \int_{-1}^1 d \cos \theta_{12} V(|\mathbf{r}_1 - \mathbf{r}_2|) P_\lambda(\cos \theta_{12}) \quad (106)$$

The non-antisymmetrized, two-nucleon matrix element between non-normalized states reads

$$V_{JM} = \langle rlj, r'l'j' | V(|\mathbf{r} - \mathbf{r}'|) | r\tilde{l}\tilde{j}, r'\tilde{l}'\tilde{j}' \rangle_{JM}, \quad (107)$$

where J and M are the total angular momentum of the two-nucleon state, and its z -projection, respectively. Since the interaction contains the spin operator, it is convenient to calculate the matrix element in the LS-coupling scheme. The transformation between the jj and LS-coupling schemes for the two nucleon state

$$|(l, l'), jj; JM\rangle = \sum_{LS} \hat{j}\hat{j}'\hat{L}\hat{S} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S \\ l & l' & L \\ j & j' & J \end{Bmatrix} |(l'l')SL; JM\rangle \quad (108)$$

where L is the total orbital angular momentum, and S the total spin of the two-nucleon state. We use the short-hand notation $\hat{j} := \sqrt{2j+1}$. The matrix element can then be written

$$V_{JM} = \sum_{LS} \sum_{\tilde{L}, \tilde{S}} \hat{j}\hat{j}'\hat{L}\hat{S}\hat{\tilde{j}}\hat{\tilde{j}}'\hat{\tilde{L}}\hat{\tilde{S}} \langle rr', (l'l')SLJM | V(|\mathbf{r} - \mathbf{r}'|) | \tilde{r}\tilde{r}', (\tilde{l}\tilde{l}')\tilde{S}\tilde{L}JM \rangle \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S \\ l & l' & L \\ j & j' & J \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \tilde{S} \\ \tilde{l} & \tilde{l}' & \tilde{L} \\ \tilde{j} & \tilde{j}' & \tilde{J} \end{Bmatrix} \quad (109)$$

Using the Slater expansion (104), the LS-coupling matrix element takes the form

$$V_{S\tilde{S}L\tilde{L}}^{JM} = \sum_{\lambda} \frac{4\pi}{2\lambda+1} V_{\lambda}(r, r') \sum_{\mu} \langle (l'l')SLJM | Y_{\lambda\mu}^*(\hat{\mathbf{r}}) Y_{\lambda\mu}(\hat{\mathbf{r}}') (A + B\hat{P}^{\sigma}) | (\tilde{l}\tilde{l}')\tilde{S}\tilde{L}JM \rangle, \quad (110)$$

where the radial factors $V_{\lambda}(r, r')$ are defined in (106), and the angular part is calculated

$$\begin{aligned} & \sum_{\mu} \langle (l'l')SLJM | Y_{\lambda\mu}^*(\hat{\mathbf{r}}) Y_{\lambda\mu}(\hat{\mathbf{r}}') (A + B\hat{P}^{\sigma}) | (\tilde{l}\tilde{l}')\tilde{S}\tilde{L}JM \rangle = \\ & \delta_{S\tilde{S}} \delta_{L\tilde{L}} (A + B(2S-1)) (-1)^{L+l+\tilde{l}} \frac{\tilde{l}\tilde{l}'\lambda^2}{4\pi} \begin{pmatrix} l & \lambda & \tilde{l} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & \lambda & \tilde{l}' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \tilde{l} & \tilde{l}' & L \\ l' & l & \lambda \end{Bmatrix} \end{aligned} \quad (111)$$

For the pairing interaction we only consider matrix elements between two-nucleon states with total angular momentum $J = 0$. In this case the $9j$ -coefficients in (109) reduce to $6j$ -coefficients, and the two-nucleon matrix element reads

$$\begin{aligned} V_{J=0} &= \delta_{jj'} \delta_{\tilde{j}\tilde{j}'} \delta_{ll'} \delta_{\tilde{l}\tilde{l}'} (2l+1)(2\tilde{l}+1) \hat{j}\hat{j}' \\ & \sum_{s=0,1} (-1)^{j+\tilde{j}+1+S} (2S+1) \begin{Bmatrix} l & l & S \\ \frac{1}{2} & \frac{1}{2} & j \end{Bmatrix} \begin{Bmatrix} \tilde{l} & \tilde{l} & S \\ \frac{1}{2} & \frac{1}{2} & \tilde{j} \end{Bmatrix} \\ & \sum_{\lambda} V_{\lambda}(r, r') (A + B(2S-1)) \begin{pmatrix} l & \lambda & \tilde{l} \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} l & \tilde{l} & \lambda \\ \tilde{l} & l & S \end{Bmatrix}. \end{aligned} \quad (112)$$

The allowed integer values for λ in the sum are

$$|l - \tilde{l}| \leq \lambda \leq l + \tilde{l} \quad (113)$$

The matrix elements essentially consist of two terms: $S = 0$ and $S = 1$. Introducing the explicit expressions for the $3j$ and $6j$ -coefficients, the two terms read

$$\begin{aligned} V_{J=0} \text{ } s=0 &= (A - B) \delta_{jj'} \delta_{\tilde{j}\tilde{j}'} \delta_{ll'} \delta_{\tilde{l}\tilde{l}'} \sum_{\lambda \text{ even}} (-1)^{\lambda} V_{\lambda}(r, r') \\ & \frac{(2g-2l)!(2g-2\lambda)!(2g-2\tilde{l})!}{2(2g+1)!} \left[\frac{g!}{(g-l)!(g-\lambda)!(g-\tilde{l})!} \right]^2 \end{aligned} \quad (114)$$

and

$$V_{J=0 \ S=1} = \frac{1}{2}(A+B)\delta_{jj'}\delta_{\tilde{j}\tilde{j}'}\delta_{ll'}\delta_{\tilde{l}\tilde{l}'}\hat{j}\hat{j}'\frac{(\frac{3}{4}+l(l+1)-j(j+1))(\frac{3}{4}+\tilde{l}(\tilde{l}+1)-\tilde{j}(\tilde{j}+1))}{l(l+1)\tilde{l}(\tilde{l}+1)}\sum_{\lambda \text{ even}}(-1)^\lambda V_\lambda(r,r')$$

$$\left[l(l+1)+\tilde{l}(\tilde{l}+1)+\lambda(\lambda+1)\right]\frac{(2g-2l)!(2g-2\lambda)!(2g-2\tilde{l})!}{2(2g+1)!}\left[\frac{g!}{(g-l)!(g-\lambda)!(g-\tilde{l})!}\right]^2 \quad (115)$$

where $2g = l + \lambda + \tilde{l}$.

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Figure Captions

- Fig. 1** Vector space homomorphisms between the general single-particle basis, the basis of quasi-particle states, and the canonical basis of single-particle states. The diagrams illustrate the transformations (15) to (17).
- Fig. 2** Relativistic Hartree-Bogoliubov model for a finite nucleus. Single-particle eigenspectrum of a Dirac hamiltonian (left and center), and single quasi-particle eigenspectrum of the Hartree-Bogoliubov equations (right).
- Fig. 3a** Occupation pattern of the global stiffness matrix \mathbf{A} (57) for $\kappa = -1$ and linear shape functions. The dark grey squares indicate matrix elements of the finite range Gogny interaction. Due to the nonlocal character of the interaction, the matrix elements are distributed over the whole matrix. The light grey squares correspond to matrix elements which result from the local operators in (36). They form a block diagonal band structure. Boundary conditions are taken into account by eliminating the corresponding rows and columns. The matrix is symmetric and we display the global index of nonzero matrix elements, as used by the bisection method in the solution of the eigenvalue problem.
- Fig. 3b** Occupation pattern of the overlap matrix \mathbf{N} (58), for $\kappa = -1$ and linear shape functions.
- Fig. 3c** Same as in Fig. 3a, but for $\kappa = +1$ and quadratic shape functions.
- Fig. 3d** Same as in Fig. 3b, but for $\kappa = +1$ and quadratic shape functions.
- Fig. 3e** Same as in Fig. 3a, but for $|\kappa| > 1$ and cubic shape functions.
- Fig. 3f** Same as in Fig. 3b, but for $|\kappa| > 1$ and cubic shape functions.
- Fig. 4a** Self-consistent normalized quasi-particle wave functions. Radial amplitudes of U-components (upper left), and V-components (upper right), for the $1s_{1/2}$ (solid), $2s_{1/2}$ (dashed), and $3s_{1/2}$ (dotted) bound states in ^{124}Sn . The radial amplitudes of continuum $s_{1/2}$ -states are shown in the lower part of the figure: U-components (left) and V-components (right). The self-consistent solution is calculated with 100 linear shape functions on a uniform radial mesh $[0, 30 \text{ fm}]$.
- Fig. 4b** Same as in figure 4a, but for $p_{1/2}$ -waves.
- Fig. 4c** Same as in figure 4a, but for $p_{3/2}$ -waves.
- Fig. 4d** Same as in figure 4a, but for $h_{11/2}$ -waves.
- Fig. 5** Baryon density of ^{124}Sn after the first iteration step (dashed), and for the self-consistent solution (solid). The results correspond to a calculation with 100 linear shape functions on a uniform radial mesh $[0, 30 \text{ fm}]$.
- Fig. 6** $\kappa = \pm 1, \pm 2, \pm 3$ contributions to the pairing field. For each value of κ we display the largest contributions from individual states. The quantities that we plot are defined in (82).
- Fig. 7** The components $\Delta^{(g)}(r)$ and $\Delta^{(f)}(r)$ of the self-consistent pairing field (82), calculated on a radial mesh of 15 fm (solid) and 30 fm (dot dashed). The pairing field is concentrated on the surface of the nucleus.
- Fig. 8** Logarithmic plots of N_n (84) and P_n (85), as functions of quasi-particle energy for the $s_{1/2}$ -states. Results are displayed for three sizes of the radial box: $r_{\text{max}} = 15 \text{ fm}$ (dashed), $r_{\text{max}} = 30 \text{ fm}$ (dot dashed) and $r_{\text{max}} = 40 \text{ fm}$ (solid).

test run	1 FEM	2 FEM	3 FEM	4 FEM	5 FEM	6 FEM	7 Osc. basis
\mathbf{r}_{\max} [fm]	15.00	20.00	30.00	40.00	20.00	20.00	
\mathbf{E}_{\max} [MeV]	100.00	100.00	100.00	100.00	70.00	110.00	
\mathbf{E}_{p} [MeV]	-1320.74	-1320.68	-1320.79	-1320.79	-1320.51	-1320.80	
\mathbf{E}_{n} [MeV]	-1719.42	-1646.68	-1719.56	-1719.56	-1719.17	-1719.54	
\mathbf{E}_{pair} [MeV]	-19.948	-19.9494	-19.9510	-19.9342	-19.5666	-19.9901	-19.68
\mathbf{E}_{sig} [MeV]	17126.70	17126.20	17126.20	17126.2	17125.30	17126.40	17432.33
\mathbf{E}_{nl} [MeV]	-324.004	-323.988	-323.983	-323.983	-324.019	-323.977	-327.910
\mathbf{E}_{ome} [MeV]	-14699.40	-14699.27	-14699.10	-14699.00	-14698.10	-14699.20	-14674.06
\mathbf{E}_{rho} [MeV]	-55.460	-55.455	-55.448	-55.448	-55.449	-55.449	-55.529
\mathbf{E}_{pho} [MeV]	-366.072	-366.072	-366.073	-366.073	-366.066	-366.075	-365.71
\mathbf{E}_{tot} [MeV]	-1060.58	-1060.69	-1060.83	-1060.82	-1055.37	-1060.86	1051.96
\mathbf{E}_b/A [MeV]	-8.553	-8.554	-8.555	-8.555	-8.550	-8.555	-8.48
λ [MeV]	-6.65727	-6.65718	-6.65706	-6.65668	-6.65719	-6.65729	-6.65786
$\mathbf{rms}_{\text{neutron}}$ [fm]	4.90853	4.90869	4.90874	4.90874	4.90825	4.90871	4.91073
$\mathbf{rms}_{\text{proton}}$ [fm]	4.59741	4.59745	4.59751	4.59741	4.59738	4.59740	4.60187
$\mathbf{rms}_{\text{nucleus}}$ [fm]	4.78555	4.78561	4.78564	4.78564	4.78515	4.78562	4.78859

Table 1 Bulk properties of ^{124}Sn . Calculated quantities are compared for various sizes of the radial mesh, and with results of an expansion in the oscillator basis [6].

test run	1	2	3	4	5	6
\mathbf{r}_{\max} [fm]	15.00	20.00	30.00	40.00	20.00	20.00
\mathbf{E}_{\max} [MeV]	100.00	100.00	100.00	100.00	70.00	110.00
$\mathbf{E}_{1s_{1/2}}$ [MeV]	-51.834	-51.834	-51.834	-51.836	-51.828	-51.832
$\mathbf{E}_{2s_{1/2}}$ [MeV]	-39.294	-39.298	-39.303	-39.300	-39.290	-39.305
$\mathbf{E}_{3s_{1/2}}$ [MeV]	-8.227	-8.231	-8.235	-8.235	-8.221	-8.235
$\mathbf{E}_{4s_{1/2}}$ [MeV]	12.988	12.997	13.050	12.902	12.981	13.085
$\mathbf{E}_{1p_{3/2}}$ [MeV]	-43.078	-43.076	-43.075	-43.077	-43.069	-43.067
$\mathbf{E}_{2p_{3/2}}$ [MeV]	-27.023	-27.029	-27.035	-27.032	-27.018	-27.043
$\mathbf{E}_{3p_{3/2}}$ [MeV]	2.977	2.969	2.961	2.961	2.983	2.965
$\mathbf{E}_{1p_{1/2}}$ [MeV]	-42.976	-42.998	-43.006	-43.008	-42.923	-43.001
$\mathbf{E}_{2p_{1/2}}$ [MeV]	-24.499	-24.489	-24.481	-24.479	-24.498	-24.486
$\mathbf{E}_{3p_{1/2}}$ [MeV]	3.863	3.850	3.843	3.842	3.894	3.849
$\mathbf{E}_{1d_{5/2}}$ [MeV]	-38.359	-38.358	-38.357	-38.357	-38.358	-38.359
$\mathbf{E}_{2d_{5/2}}$ [MeV]	-10.678	-10.683	-10.686	-10.686	-10.671	-10.685
$\mathbf{E}_{3d_{5/2}}$ [MeV]	13.245	13.265	13.271	13.218	13.203	13.283
$\mathbf{E}_{1d_{3/2}}$ [MeV]	-35.690	-35.691	-35.692	-35.692	-35.681	-35.693
$\mathbf{E}_{2d_{3/2}}$ [MeV]	-8.489	-8.494	-8.496	-8.497	-8.471	-8.496
$\mathbf{E}_{3d_{3/2}}$ [MeV]	13.851	13.887	14.051	13.801	13.766	14.096
$\mathbf{E}_{1g_{7/2}}$ [MeV]	-16.971	-16.970	-16.969	-16.969	-16.998	-16.969
$\mathbf{E}_{2g_{7/2}}$ [MeV]	11.400	11.512	11.557	11.551	11.289	11.466
$\mathbf{E}_{1h_{11/2}}$ [MeV]	-6.349	-6.348	-6.347	-6.347	-6.355	-6.347
$\mathbf{E}_{2h_{11/2}}$ [MeV]	22.127	22.116	22.107	22.110	22.138	22.212
$\mathbf{v}_{1s_{1/2}}^2$	0.999995	0.999995	0.999995	0.999995	0.999995	0.999995
$\mathbf{v}_{2s_{1/2}}^2$	0.999598	0.999596	0.999594	0.999594	0.999611	0.999593
$\mathbf{v}_{3s_{1/2}}^2$	0.984564	0.984573	0.984585	0.984603	0.984593	0.984558
$\mathbf{v}_{4s_{1/2}}^2$	0.000048	0.000048	0.000049	0.000049	0.000046	0.000049
$\mathbf{v}_{1p_{3/2}}^2$	0.999900	0.999900	0.999899	0.999899	0.999835	0.999899
$\mathbf{v}_{2p_{3/2}}^2$	0.998427	0.998419	0.998413	0.998414	0.998483	0.998410
$\mathbf{v}_{3p_{3/2}}^2$	0.000499	0.000503	0.000505	0.000504	0.000413	0.000506
$\mathbf{v}_{1p_{1/2}}^2$	0.999941	0.999940	0.999939	0.999939	0.999964	0.999939
$\mathbf{v}_{2p_{1/2}}^2$	0.999025	0.999019	0.999015	0.999016	0.999082	0.999013
$\mathbf{v}_{3p_{1/2}}^2$	0.000218	0.000219	0.000220	0.000220	0.000203	0.000221
$\mathbf{v}_{1d_{5/2}}^2$	0.999205	0.999200	0.999198	0.999198	0.999256	0.999195
$\mathbf{v}_{2d_{5/2}}^2$	0.987226	0.987186	0.987160	0.987166	0.987347	0.987134
$\mathbf{v}_{3d_{5/2}}^2$	0.000135	0.000135	0.000136	0.000135	0.000128	0.000137
$\mathbf{v}_{1d_{3/2}}^2$	0.999384	0.999381	0.999379	0.999378	0.999421	0.999376
$\mathbf{v}_{2d_{3/2}}^2$	0.966344	0.966348	0.966337	0.966350	0.966473	0.966276
$\mathbf{v}_{3d_{3/2}}^2$	0.000095	0.000095	0.000096	0.000096	0.000077	0.000097
$\mathbf{v}_{1g_{9/2}}^2$	0.992754	0.992711	0.992680	0.992687	0.992934	0.992660
$\mathbf{v}_{2g_{9/2}}^2$	0.000410	0.000415	0.000417	0.000417	0.000352	0.000419